

Contribution of Berry Curvature to Thermoelectric Effects

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Within the semiclassical Boltzmann transport theory, the formula for Seebeck coefficient S is derived for an isotropic two-dimensional electron gas (2DEG) system that exhibits anomalous Hall effect (AHE) and anomalous Nernst effect (ANE) originating from Berry curvature on their bands. Deviation of S from the value S_0 estimated neglecting Berry curvature is computed for a special case of 2DEG with Zeeman and Rashba terms. The result shows that, under certain conditions the contribution of Berry curvature to Seebeck effect could be non-negligible. Further study is needed to clarify the effect of additional contributions from mechanisms of AHE and ANE other than pure Berry curvature.

KEYWORDS: thermoelectric effect, anomalous Hall effect, anomalous Nernst effect, Berry curvature, two-dimensional electron gas

1. Introduction

Thermoelectric effects, the mutual conversion of heat and electricity in materials, have been attracting much attention these days due to their great potential for applications such as eco-friendly power generation from waste heat, or Peltier cooler for small devices. Much efforts have been made to find materials with better efficiency of conversion achieved by larger value of $Z = \sigma S^2 / \kappa$, where σ , S , κ are longitudinal electrical conductivity, Seebeck coefficient, and thermal conductivity, respectively. We now have, based on those works, some guides in the quest for better materials, among which are the low dimensionality of the system, expected to make σ large while keeping the magnitude of S [1], or some specific structures which are believed to suppress thermal conduction efficiently.

What we present in this paper is another ingredient, namely the transverse components σ_{xy} and α_{xy} of the tensors $\tilde{\sigma}$, $\tilde{\alpha}$ in the expression of charge current $\mathbf{j} = \tilde{\sigma}\mathbf{E} + \tilde{\alpha}(-\nabla T)$, where \mathbf{E} and ∇T are electric field and temperature gradient, respectively. These transverse components naturally participate in the determination of longitudinal quantity S as will be seen in the formula in the following section. As to the origin of σ_{xy} and α_{xy} , one can think of either external magnetic field or spontaneous magnetization. An example of the former is seen in [2], where two-dimensional electron gas (2DEG) in a quantizing magnetic field was studied. In what follows our target is the latter. These effects, the appearance of σ_{xy} and α_{xy} in zero magnetic field, are called anomalous Hall effect (AHE) [3] and anomalous Nernst effect (ANE) [4], respectively. Their origins had been a controversial problem for many decades, but it was shown both experimentally [5, 6] and theoretically [7–10] that for some cases so-called intrinsic contribution becomes important. It stems purely from some band structures and in the clean limit, the conductivities are expressed, as we will review in the following section, as a functional of Berry curvature $\Omega(\mathbf{k}) \equiv i\langle \partial_{\mathbf{k}} u | \times | \partial_{\mathbf{k}} u \rangle$, where $|u_{\mathbf{k}}\rangle$ is the periodic part of a Bloch

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state. Various topics related to Berry curvature are reviewed in Ref. [4]. The target of the present study is to roughly estimate how much this intrinsic contribution could affect the value of Seebeck coefficient in the case of 2DEG, the systems promising for thermoelectric applications due to its low dimensionality.

2. Derivation of the formula for Seebeck coefficient

We derive below the semiclassical formula for Seebeck coefficient. The starting point is the expression for charge current \mathbf{j} obtained in Ref. [11], which reads,

$$\mathbf{j} = e \int \frac{d\mathbf{k}}{(2\pi)^2} g(\mathbf{r}, \mathbf{k}) \mathbf{v}_{\mathbf{k}} + e \nabla_{\mathbf{r}} \times k_B T(\mathbf{r}) \int \frac{d\mathbf{k}}{(2\pi)^2} \boldsymbol{\Omega}(\mathbf{k}) \log \left[1 + \exp \left(-\frac{\varepsilon_{\mathbf{k}} - \mu}{k_B T(\mathbf{r})} \right) \right], \quad (1)$$

where e , $g(\mathbf{r}, \mathbf{k})$, $T(\mathbf{r})$, $\mathbf{v}_{\mathbf{k}}$, $\varepsilon_{\mathbf{k}}$, and μ stand for the electron's charge ($e < 0$), distribution function, local temperature, velocity and energy of an electron with wave number \mathbf{k} and chemical potential, respectively. Hereafter we use atomic units ($\hbar = 1$, $|e| = 1$, $m = 1$) unless explicitly specified.

The second term is a correction that appears when spatial inhomogeneity (i.e., $T(\mathbf{r})$ in the present case) exists. Simplifying the second term following Ref. [11] and substituting the equation of motion of a perturbed (by \mathbf{E} field) Bloch electron

$$\mathbf{v}_{\mathbf{k}} = \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}), \quad (2)$$

which was derived in Ref. [12], for $\mathbf{v}_{\mathbf{k}}$ and the form of distribution

$$g(\mathbf{r}, \mathbf{k}) = \tau_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \cdot \left[e \mathbf{E} + (\varepsilon_{\mathbf{k}} - \mu) \left(-\frac{\nabla T}{T} \right) \left(-\frac{\partial f}{\partial \varepsilon} \right) \right], \quad (3)$$

obtained as the solution of Boltzmann transport equation within relaxation time ($\tau_{\mathbf{k}}$) approximation, for $g(\mathbf{r}, \mathbf{k})$, we obtain

$$\begin{cases} \sigma_{xx} = \frac{e^2 \tau}{2} \int d\varepsilon D(\varepsilon) v_0(\varepsilon)^2 \left(-\frac{\partial f}{\partial \varepsilon} \right) = \sigma_{yy}, \\ \sigma_{xy} = -e^2 \int d\varepsilon D(\varepsilon) \Omega_z(\mathbf{k}) = -\sigma_{yx}, \\ \alpha_{ij} = \frac{1}{e} \int d\varepsilon \sigma_{ij}(\varepsilon)_{T=0} \frac{\varepsilon - \mu}{T} \left(-\frac{\partial f}{\partial \varepsilon} \right) \quad \text{for } i = x \text{ or } y, j = x \text{ or } y, \end{cases} \quad (4)$$

where $D(\varepsilon)$ and $v_0(\varepsilon) \equiv d\varepsilon(k)/dk$ are density of states and electron's group velocity, respectively. We restricted ourselves to the case of isotropic 2DEG, i.e., $\varepsilon(\mathbf{k}) = \varepsilon(k)$, $\boldsymbol{\Omega} = (0, 0, \Omega_z)$ and assumed constant relaxation time ($\tau_{\mathbf{k}} = \tau$).

The formula for thermoelectric coefficients follow immediately by substituting Eq. (4) for $\tilde{\sigma} = [\sigma_{ij}]$ and $\tilde{\alpha} = [\alpha_{ij}]$ in the linear response relation $\mathbf{j} = \tilde{\sigma} \mathbf{E} + \tilde{\alpha} (-\nabla T)$. The result is,

$$\begin{cases} S \equiv S_{ii} \equiv \frac{E_i}{\partial_i T} = \frac{\alpha + \beta \gamma}{1 + \beta^2} \quad \text{for } i = x \text{ or } y \\ N \equiv S_{xy} \equiv \frac{E_x}{\partial_y T} = \frac{\gamma - \alpha \beta}{1 + \beta^2} = -S_{yx}. \end{cases} \quad (5)$$

Here we defined $\alpha \equiv \alpha_{xx}/\sigma_{xx}$, $\beta \equiv \sigma_{xy}/\sigma_{xx}$, $\gamma \equiv \alpha_{xy}/\sigma_{xx}$ for a simpler notation.

Note that the Seebeck coefficient S_0 estimated without considering Berry curvature is obtained by setting $\beta = 0$ and $\gamma = 0$ in Eq. (5), i.e. $S_0 = \alpha$.

3. Model

Next we estimate how much S could deviate from S_0 according to Eq.(5). We choose here, as an example system, Zeeman-Rashba 2DEG (ZR2DEG) most simply described by the following Hamiltonian:

$$H = \frac{k^2}{2m^*} + \lambda(\mathbf{e}_z \times \mathbf{k}) \cdot \boldsymbol{\sigma} - \Delta\sigma_z \equiv \frac{k^2}{2m^*} + \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (6)$$

where m^* , λ , \mathbf{e}_z , $\boldsymbol{\sigma}$, Δ , and $\mathbf{h}(\mathbf{k}) \equiv (-\lambda k_y, \lambda k_x, -\Delta)$ are the effective mass of an electron, Rashba parameter, unit vector normal to the 2DEG plane (which we take to be xy -plane), spin operator, exchange field for an electron, and effective "magnetic field", respectively. Rashba term, the second one, is a spin-orbit coupling originating from the structural inversion asymmetry, which is present on the surface or at the interface of layers [13]. The parameter λ is determined not only by the kind of material but is tunable with an applied gate-voltage [14, 15]. Zeeman term, the last one, is assumed here to represent an exchange field created by localized spins at magnetic impurities and felt by a spin of Bloch electron. Thus we here regard the Hamiltonian above as a model of 2DEG, induced for example at the interface of a semiconductor heterostructure doped with magnetic impurities such as Mn. Note, however, that Eq.(6) has been studied not only as a model for 2DEG but also as a minimum model of 2D partial structure of 3D ferromagnetic metals accompanying Berry curvature [3, 4, 8, 10]. This system has eigenstates

$$|u_-\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix}, \quad |u_+\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix}, \quad (7)$$

where the angles $\theta = \theta(\mathbf{k})$ and $\phi = \phi(\mathbf{k})$ are those of polar coordinates of the vector $\mathbf{h}(\mathbf{k})$, and the corresponding eigenenergies are

$$\varepsilon_{\pm} = \frac{k^2}{2m^*} \pm \sqrt{\lambda^2 k^2 + \Delta^2}. \quad (8)$$

Each band has the Berry curvature

$$\Omega(\mathbf{k})_{\pm} = \left(0, 0, \mp \frac{\lambda^2 \Delta}{2(\lambda^2 k^2 + \Delta^2)^{3/2}} \right). \quad (9)$$

Note that, in our model, the absence of either term, Zeeman (time-reversal symmetry (TRS) breaking) or Rashba (inversion symmetry (IS) breaking), leads to zero Berry curvature, although in general, finite curvature is allowed in the presence of either TRS or IS.

We plot Eq.(8) and Eq.(9) in Fig.(1) for some values of parameters. We use hereafter $\eta \equiv m^* \lambda^2 / \Delta$ instead of λ , since η nicely controls the shape of ε_- band (i.e., $\eta = 1$ is a critical value between ε_- bands with topologically different Fermi surfaces) and in addition, all conductivities we need become independent of m^* once we fix the values of the pair η and Δ .

According to Ref. [14] the value of λ ranges from at most 0.69 meV·nm for GaAs to at least 100 meV·nm for HgMnTe. For Δ , example values of 25 meV and 122 meV for (Ga,Mn)As are found in Ref. [7].

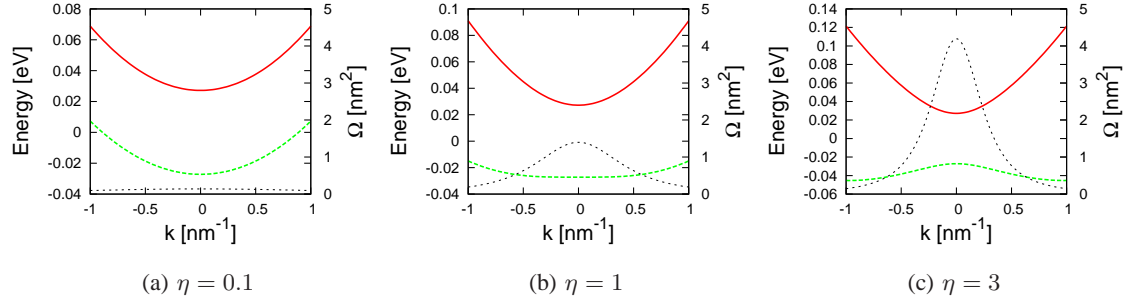


Fig. 1. (Color online) Band dispersions(left axis, red: ε_+ , green: ε_-) and Berry curvature(right axis, black broken) of ZR2DEG plotted as a function of wave number $k = |\mathbf{k}|$. $m^* = 1$, $\Delta = 10^{-3}$

4. Results and Discussions

Seebeck coefficient was calculated numerically for wide range of parameters using Eq.(5). First of all, the relative deviation of S , the Berry curvature-included value, from conventionally estimated S_0 , evaluated by $r \equiv (S - S_0)/S_0$, becomes relatively large when (i) band parameter η is of order 1 to 10, and (ii) chemical potential μ is situated near the ε_- band edge.

These trends (i) and (ii) can be understood qualitatively as follows: (i) $\eta \simeq 1$ means large density of states near the ε_- band edge, where $\Omega(k)$ has its peak, leading to the grow of σ_{xy} and α_{xy} . (ii) Low μ suppresses σ_{xx} and thus make β and γ large.

We therefore concentrate on some points in such parameter region and show the temperature dependence and relaxation time dependence there in Fig.(2).

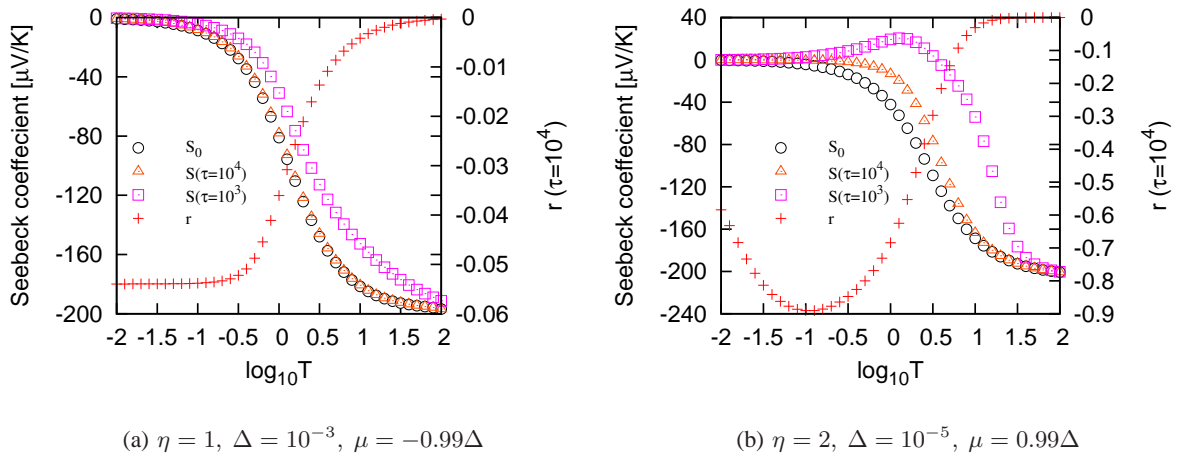


Fig. 2. (Color online) Temperature dependence of Seebeck coefficients (left axis) S_0 (circle), S for $\tau = 10^4$ (square, pink) and $\tau = 10^3$ (rotated square, blue) and of the relative strength of anomaly r (right axis, plus sign, red) for $\tau = 10^4$.

Fig.2 (a) is a plot for the case of $\eta = 1$ (the special point as pointed out above), $\Delta = 10^3$, and the chemical potential μ situated only one hundredth of Δ above the ε_- band edge. One cannot distinguish, on the plotted scale, S for $\tau = 10^5$ (rather clean case, not shown in figure) from S_0 . For 10 times dirtier case ($\tau = 10^4$), the absolute value of r , by which we evaluate the extent of anomaly, reaches $\simeq 4\%$ around $T \simeq 1\text{K}$. Further increase in the scattering strength ($\tau = 10^3$) makes the anomaly much larger in a wider range of T .

Fig.2 (b) is plotted for $\eta = 2$ (of the same order as Fig.2 (a)), 100 times smaller exchange Δ compared to Fig.2 (a), and μ put at $\mu = 0.99\Delta$. The general dependence on τ is similar to that in Fig.2 (a), except that for $\tau = 10^3$, S varies non-monotonically with T and even shows hole-like sign $S > 0$ in lower T range.

Regarding both (a) and (b) in Fig.2, one recognizes that in all cases (considering Berry curvature or not, and independent of the value of τ), Seebeck coefficient approaches to zero as T is lowered, in consistent with well-known Mott's law. On the high T side, S values are converging into S_0 , which is because σ_{xx} and α_{xx} increase as a function of T at least at a faster rate than their transverse counterparts (The latter ones even begin to decay at some T in the plotted range as T increases in the case of Fig.2 (b)). The reason is that, due to its small split $\Delta \approx k_B T$ at $T \approx 1\text{K}$, smoothed function $f(\varepsilon)$ suppresses σ_{xy} by causing cancellation of $\pm\Omega$ on each band and that broadened function $\partial f/\partial\varepsilon$ inhibits the grow of α_{xy} .

The above mentioned trend regarding τ is predictable from the explicit relations $\beta \propto \tau^{-1}$, $\gamma \propto \tau^{-1}$ (see the definitions in Section 2.). However, we have to be careful regarding this result, since shorter τ means worse defined quantum number \mathbf{k} . There is also a possibility that it is necessary to take into account extrinsic scattering-related mechanisms of AHE and ANE by applying techniques such as intuitive semiclassical theories (that include many other contributions than ours with only the intrinsic one) or more rigorous quantum theories (Kubo-Streda formula or Keldysh formalism).

5. Summary

The semiclassical formula for Seebeck coefficient that includes the contribution of Berry curvature was derived. For a special case of Zeeman-Rashba 2DEG, the following result was obtained: When (i) the temperature is rather low, (ii) scattering is not too weak, and (iii) the band shape has some specific feature, Berry curvature could have quite large effect on Seebeck coefficient. It is to be studied to what extent extrinsic AHE and ANE modify our results.

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